Electrostatic Comparison of Biomolecular Structures

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Electrostatic interactions play an important role in many biological processes, often controlling the affinity and specificity of biomolecular interactions. The electrostatic properties of a biomolecule are determined by both its fold and amino acid composition, therefore leading to characteristics which combine both structure and sequence. Given these facts, it is not surprising that electrostatic data has been used, with varying degrees of success, to compare and classify proteins. In this poster, we describe several new topological metrics and analysis methods to efficiently and robustly characterize the electrostatic properties of biological macromolecules. Specifically, we examine the ability of critical point methods to capture the necessary details of electrostatic potentials and then use several clustering methods to classify the biomolecular structures according to the traditional and the new topological metrics. Additionally, we describe the application of the highly-scalable APBS software (http://agave.wustl.edu/apbs) to rapidly characterize electrostatic potentials for large sets of biomolecular structures. These methods are applied to a large set of protein families with very different folds and sequences to demonstrate the relative abilities of the various metrics, both new and old, to cluster the proteins into appropriate families and classes. The resulting classification is then compared against a number of existing structure-, sequence-, and function-based groupings, including: SCOP, Pfam, simple sequence similarity, and the EC system. Finally, we discuss future directions for electrostatic comparison methods and their potential application to other systems.